1(a). \[ \mathbf{V}(\mathbf{x}) = \text{pot. energy of one spring as fun. of length.} \]

\[ l_\alpha = | \overrightarrow{\mathbf{m}} - \overrightarrow{\mathbf{x}_\alpha} | = \text{dist from m to corner } \alpha. \]

\[ \mathbf{V}(\mathbf{x}) = \sum_{\alpha=1}^{3} \mathbf{V}(l_\alpha). \]
Want \( V''_{ij} = \frac{\partial^2 V}{\partial x_i \partial x_j} (0) \). Group theory says this is a multiple of identity.

\[
\frac{\partial V}{\partial x_i} = \sum_{\alpha = 1}^{3} \nu' (l_{\alpha}) \frac{\partial l_{\alpha}}{\partial x_i}
\]

\[
\frac{\partial^2 V}{\partial x_i \partial x_j} = \sum_{\alpha} \left( \nu'' (l_{\alpha}) \frac{\partial l_{\alpha}}{\partial x_i} \frac{\partial l_{\alpha}}{\partial x_j} + \nu' (l_{\alpha}) \frac{\partial^2 l_{\alpha}}{\partial x_i \partial x_j} \right).
\]

\[
\frac{\partial l_{\alpha}}{\partial x_i} = \frac{x_i - C_{\alpha i}}{|\vec{x} - \vec{C}_{\alpha}|},
\]

\[
\frac{\partial^2 l_{\alpha}}{\partial x_i \partial x_j} = \frac{\delta_{ij}}{|\vec{x} - \vec{C}_{\alpha}|} - \frac{(x_i - C_{\alpha i})(x_j - C_{\alpha j})}{|\vec{x} - \vec{C}_{\alpha}|^3}.
\]

Now evaluate at \( \vec{x} = 0 \), where \( l_{\alpha} = a \) (all \( \alpha \)).

\[
\frac{\partial l_{\alpha}}{\partial x_i} (0) = \frac{-C_{\alpha i}}{a}
\]

\[
\frac{\partial^2 l_{\alpha}}{\partial x_i \partial x_j} (0) = \frac{\delta_{ij}}{a} - \frac{C_{\alpha i} C_{\alpha j}}{a^3}
\]

\[
\frac{\partial V}{\partial x_i} (0) = \sum_{\alpha} \nu' (a) \left( \frac{-C_{\alpha i}}{a} \right) = -\frac{\nu' (a)}{a} \sum_{\alpha} C_{\alpha i} = 0
\]

because \( \sum_{\alpha} C_{\alpha} = 0 \). (Cond. that \( \vec{x} = 0 \) is an equilibrium).

\[
\frac{\partial^2 V}{\partial x_i \partial x_j} (0) = \sum_{\alpha} \left[ \nu'' (a) \frac{C_{\alpha i} C_{\alpha j}}{a^2} + \nu' (a) \left( \frac{\delta_{ij}}{a} - \frac{C_{\alpha i} C_{\alpha j}}{a^3} \right) \right]
\]
\[ \frac{\partial^2 V}{\partial x_i \partial x_j} (0) = \frac{3}{a} v'(a) \delta_{ij} + \left( \frac{v''(a)}{a^2} - \frac{v'(a)}{a^3} \right) \sum_{\alpha} C_{\alpha i} C_{\alpha j}. \]

Do this a multiple of the identity? Look 1st at off diag. element.

Of 2nd term.

\[ \sum_{\alpha} C_{\alpha x} C_{\alpha y} = a^2 \left[ (0)(1) + (-\frac{\sqrt{3}}{2})(-\frac{1}{2}) + (+\frac{\sqrt{3}}{2})(-\frac{1}{2}) \right] = 0. \]

Yes.

Now see if diag. terms are equal.

\[ \sum_{\alpha} C_{\alpha x}^2 = a^2 \left[ 0 + \frac{3}{4} + \frac{3}{4} \right] = \frac{3}{2} a^2 \]

\[ \sum_{\alpha} C_{\alpha y}^2 = a^2 \left[ 1 + \frac{1}{4} + \frac{1}{4} \right] = \frac{3}{2} a^2. \]

So, \[ \sum_{\alpha} C_{\alpha i} C_{\alpha j} = \frac{3}{2} a^2 \delta_{ij}, \quad \text{and} \]

\[ \frac{\partial^2 V}{\partial x_i \partial x_j} (0) = \frac{3}{2} \left[ \frac{v'(a)}{a} + v''(a) \right] \delta_{ij}. \]

QED, it's a multiple of identity.

Note: if \( \delta_{ij} > 0 \) is a stable equal., then the coef. of \( \delta_{ij} \) must be > 0.

Suppose the spring obeys Hooke's law, \( v(x) = \frac{1}{2} k x^2, \ k > 0 \).

Then \( v''(a) = k, \ \ v'(a) = ka, \ \ \text{and} \)

\[ \frac{\partial^2 V}{\partial x_i \partial x_j} = \frac{3}{2m} \left( \frac{v'(a)}{a} + v''(a) \right). \]

So the (degenerate) frequency is \( \omega = \sqrt{\frac{3}{2m} \left( \frac{v'(a)}{a} + v''(a) \right)}. \)
(b) Need characters of 3D rep. of \( D_{3h} \). There are 6 classes.

\[
\begin{align*}
\text{Class} & \\
E: & \quad \chi = 3 \\
\sigma_h & = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \chi = 1 \\
2C_3, \ e.g. & \quad R_1 = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \chi = 0 \\
2S_3, \ e.g. & \quad \sigma_h R_1 = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \chi = -2 \\
3C_2, \ e.g. & \quad R_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \chi = -1 \quad R(\hat{\gamma}, \pi) \\
3 \sigma_v, \ e.g. & \quad \sigma_v R_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{pmatrix}, \quad \chi = +1 \\
\end{align*}
\]

Summary:

<table>
<thead>
<tr>
<th></th>
<th>( E )</th>
<th>( \sigma_h )</th>
<th>( 2C_3 )</th>
<th>( 2S_3 )</th>
<th>( 3C_2 )</th>
<th>( 3\sigma_v )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 3 \mathbf{D} )-rep. ( \rightarrow ) ( \chi )</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>-2</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

Now use character orthogonality relations, you find...

\[
\text{\( 3\mathbf{D} \)-rep of} \quad D_{3h} = A_4 \oplus E_2
\]
so we have one nondegen. $\omega^{A+}$ and one 2-fold degen $\omega^{E_2}$.

It's a good guess that the $A_4$ mode is oscillation in the $z$-direc.
and the degen $E_2$ modes are in the $x$-$y$ plane.

2. The $9D$ rep. of $D_{3h}$ is made up of blocks containing either 0 or copies
of the $3D$ rep of $D_{3h}$. See p. 13, 3/19/03 for how this worked out in the
case of $C_{3v}$ (but there the blocks were $2x2$).

Write $R_n$, $n = 0, 1, \ldots, 5$ for the 6 $3x3$ rotations of $D_3$,
and then set

\[
R_0 = \mathbb{1} \qquad R_5 = \sigma_z \qquad R_6 = \sigma_h \qquad R_7 = \sigma_v \qquad R_1 = \sigma_{vz} \qquad R_{11} = \sigma_{vz}
\]

for the remaining 6 rotations (all improper). Write $R^{(9)}$ for
the $9D$ rep. For example,

\[
R^{(9)}_{1} = \begin{pmatrix}
0 & 0 & R_1 \\
R_1 & 0 & 0 \\
0 & 0 & R_1
\end{pmatrix}
\]
e.t. just like on p. 13, 3/19/03.

We need the characters of the $9D$ rep., $\chi^{(9)}$ call them. Use the
rule on p. 14, 3/19/03: $\chi^{(9)}_m$ is $\chi^{(3)}_m$ (char of $3x3$ rep) times
number of masses whose positions are left invariant by $R_n$. 

5
Make a table:

<table>
<thead>
<tr>
<th>class</th>
<th>E</th>
<th>$\sigma_u$</th>
<th>2$C_3$</th>
<th>2$S_2$</th>
<th>3$C_2$</th>
<th>3$S_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td># masses left unmoved</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$\chi^{(A)}$</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>-2</td>
<td>-1</td>
<td>+1</td>
</tr>
<tr>
<td>$\chi^{(A2)}$</td>
<td>9</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

Use char. orthog. relations, you find,

$$
QD_{rep} = A_1 \oplus A_2 \oplus A_4 \oplus E_1 \oplus 2E_2
$$

d of $D_{3h}$

So there are the following frequencies:

- $\omega^{A_1}
- \omega^{A_2}$ non-degen.
- $\omega^{A_4}$
- $\omega^{E_1}$ 2-fold degen.
- $\omega^{E_2_1}$, $\omega^{E_2_2}$ 2-fold degen.

(group theoretical analysis of the vibrational modes of the 6-spring, 3-mass problem.)
Useful notes on the characters of elements of $O(3)$.

If $R \in O(3)$, then either $\det R = +1$ (proper) or $\det R = -1$ (improper).
First take case $\det R = +1$ (proper). Then every such $R$ can be written in axis-angle form,

$$R_{\text{prop}} = R(\hat{n}, \theta)$$

Note, $R_{\text{prop}} \hat{n} = \hat{n}$,

so $\hat{n}$ is an eigenvector of $R_{\text{prop}}$ with eigenvalue $+1$. Geometrically,
$R(\hat{n}, \theta)$ rotates vectors in the plane $\perp \hat{n}$ as a 2D rotation, and
does nothing to the axis. So to compute the trace, go to a frame
where $\hat{n} = \hat{z}$ and $\hat{x}, \hat{y}$ span the plane $\perp \hat{n}$. Then

$$R_{\text{prop}} = \begin{pmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix}$$

and $X(\theta) = tr R(\hat{n}, \theta) = 2 \cos \theta + 1$.
The character is indep. of $\hat{n}$.

Now take case of improper rotation, $R_{\text{imp}} \in O(3)$, $\det(R_{\text{imp}}) = -1$.
Then you can show that there exists an axis $\hat{n}$ and angle $\theta$
such that

$$R_{\text{imp}} = \mathcal{T}_n R(\hat{n}, \theta),$$

where $\mathcal{T}_n$ means reflection in plane $\perp \hat{n}$. Note that

$$\mathcal{T}_n R(\hat{n}, \theta) = R(\hat{n}, \theta) \mathcal{T}_n.$$
\( R(\hat{n}, \theta) \)

because \( \hat{n} \) only affects vectors in the \( z \) plane, and \( \sigma_z \) only affects vectors parallel to \( \hat{n} \).

Note also, \( R_{\text{imp}} \hat{n} = \sigma_z R(\hat{n}, \theta) \hat{n} = \sigma_z \hat{n} = -\hat{n} \), so \( \hat{n} \) is an eigenvector of \( R_{\text{imp}} \) with eigenvalue \(-1\).

Now in the same coordinate system,

\[
R_{\text{imp}} = \begin{pmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & -1
\end{pmatrix},
\]

so

\[
X(\theta) = 2 \cos \theta - 1 \quad \text{for improper rotations.}
\]

**Summary:** For \( R \in O(3) \),

<table>
<thead>
<tr>
<th>General form of ( R )</th>
<th>Character ( X(\theta) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>proper ( R(\hat{n}, \theta) )</td>
<td>( 2 \cos \theta + 1 )</td>
</tr>
<tr>
<td>improper ( \sigma_z R(\hat{n}, \theta) )</td>
<td>( 2 \cos \theta - 1 )</td>
</tr>
</tbody>
</table>
Now we go back to the general theory.

See p. 17, 2/19/03.

1. Motivation for next step: Use group theory to get the normal modes of vibration, not just degeneracies of frequencies. (Still thinking of spring problems.)

2. Want to review what happens when a matrix (like $V$ in the spring problem or a Hamiltonian matrix in QM) commutes with a representation of a group. We discussed this previously in terms of blocks of matrices; see pp. 10-11, 3/5/03. Now we'll like to look at same question again, from standpoint of symmetry adapted basis.
adapted basis.

The vectors of the symmetry adapted basis (S.A.B.) are labelled by 3 indices:

\[ \begin{align*}
\tau &= \text{irrep label} \\
\alpha &= \text{number of the copy of } \tau = 1, ..., \chi_{\tau} \\
i &\quad \text{label of row or column within a single} \\
&\quad \text{copy of } \tau = 1, ..., d_{\tau}
\end{align*} \]

I will call the basis vectors of the SAB \( \{ e^{\tau i} \} \). I will also call them \( \{ l_{\tau \alpha i} \} \) using Dirac notation. I have preferred not to use Dirac notation because the vectors in question are not necessarily wavefunctions or states of a quantum system, but I think it is convenient for the next few steps. Thus in the following,

\[ ( e^{\tau i}, T(g) e^{sj} ) \quad \text{and} \quad \langle \tau \alpha i \mid T(g) \mid s \beta j \rangle \]

mean the same thing.

Now I want to go over again the material presented earlier (see pp. 2-4 and 9-12 of 31/5/03) regarding the form of a matrix \( \iota_{\tau \alpha} \) of an operator that commutes with a representation of a group (generally reducible), but do it from the standpoint of the SAB \( \{ e^{\tau i} \} \) or \( \{ l_{\tau \alpha i} \} \).

So suppose we have an operator \( H \) such that \( (H : V \rightarrow V) \)

\[ T(g) H = H T(g) , \quad \text{all } g \in G. \]

We will express this in the SAB. First look at matrix elements
of \( T(g) \) in the SAB (i.e. the matrix \( M(g) \) on p. 17):

\[
\langle rai | T(g) | s\beta j \rangle = \delta_{rs} \delta_{\alpha\beta} M_{ij}^{(r)}(g).
\]

This equation just expresses the diagonal block structure seen on p. 17, 3/19/03. Now put \( T(g) H = H T(g) \) into matrix form:

\[
\langle rai | T(g)H | s\beta j \rangle = \langle rai | H T(g) | s\beta j \rangle
\]

and insert a resolution of the identity,

\[
1 = \sum_{tyk} |tyk\rangle \langle tyk|.
\]

Then

\[
\text{LHS} = \sum_{tyk} \langle rai | T(g) | tyk \rangle \langle tyk | H | s\beta j \rangle
\]

\[
= \sum_{tyk} \delta_{rt} \delta_{\alpha\gamma} M_{ik}^{(r)}(g) \langle tyk | H | s\beta j \rangle = \sum_{k} M_{ik}^{(r)}(g) \langle rai | H | s\beta j \rangle
\]

\[
\text{RHS} = \sum_{tyk} \langle rai | H T(g) | tyk \rangle \langle tyk | T(g) | s\beta j \rangle
\]

\[
= \sum_{tyk} \langle rai | H | tyk \rangle \delta_{ks} \delta_{\gamma\beta} M_{kj}^{(s)}(g) = \sum_{k} \langle rai | H | s\beta k \rangle M_{kj}^{(s)}(g).
\]

Or if we define the \( dx \times ds \) matrix:

\[
H_{ij}^{\alpha, \beta} = \langle rai | H | s\beta j \rangle
\]
then

\[ M^{(s)}(g) H^{r, s \beta} = H^{r, s \beta} M^{(s)}(g) \]

or, by Schur's lemma, \( H^{r, s \beta} = 0 \) unless \( r = s \), in which case it is a multiple of the identity,

\[ H^{r, s \beta} = \delta_{rs} h^{\alpha \beta} I, \quad h^{\alpha \beta} = \text{a number} \]

where \( I = d_r \times d_r \) identity. Or, in components, this is

\[ \langle r a i | H | s j \alpha \beta \rangle = \delta_{rs} \delta_{ij} h^{\alpha \beta} \]

\( \delta_{rs} \) means \( H \) does not connect subspaces belonging to 2 different irreps.

\( \delta_{ij} \) means that it is a multiple of the identity when connecting two copies \((s, \beta)\) of a given irrep.

\( h^{\alpha \beta} \) is the multiple of the identity (which depends on the copies in question).

---

Next subject: The phrase "transforms as".

Context is same as above: We have a rep. \( g \rightarrow T(g) \) of a group by means of unitary operators \( T(g) : V \rightarrow V \). We do not assume \( T(g) \) is irreducible. The space \( V \) may be large. Think of the 9D rep. of \( C_3v \) in the six-spring problem.

Suppose we have a set of vectors, \( \{ x_j \in V! \; j = 1, \ldots, d_r \} \)

such that

\[ T(g) x_i = \sum_j x_j M_{ji}^{(r)}(g) \]
Then we say the set \( \{ x_i \} \) transforms as the \( r \)-th irrep of the group.

**Example:** The vectors of the symmetry adapted basis:

\[
T(g) |x_i\rangle = \sum_{\beta j} 1_{\beta j} \langle x_{\beta j} | T(g) |x_i\rangle \\
\sum_{\beta j} 1_{\beta j} \delta_{\beta \beta} \exp M_{\beta i}^{(r)}(g)
\]

because of block diagonal form.

So the S.A.B. vectors within one copy of one irrep transform as that irrep.

**2nd Example:** Suppose a vector transforms as the trivial irrep. This is 1D, so you don't need the index on \( x_i \); just write \( x \). If a vector \( x \) transforms as the trivial irrep, then

\[
T(g) x = x M^{(\text{triv})}_{11}(g).
\]

But \( M^{(\text{triv})}(g) = \begin{pmatrix} 1 & \mathbf{0} \\
\mathbf{0} & \mathbf{1} \end{pmatrix} \) because of \( 1 \times 1 \) matrix

So \( T(g) x = x \) in trivial irrep.

The vector \( x \) is invariant under the group if it transforms as the trivial irrep. Thus we call it a scalar.

[It may seem strange to call a vector a scalar, but there are different meanings to the word "vector." For example, the potential \( V \) in the spring problems is invariant under the group, hence a scalar, but it is also a member of the vector space of functions on configuration space.]
Now to projection operators. Same context as above, a rep of a group, 
$g \mapsto T(g)$, where $T(g): V \to V$. It turns out we can define projection 
operators onto the various subspaces of $V$ that transform as the different 
irreps of the group. For example, the $r$-th such subspace is the one 
spanned by $|r\alpha_i\rangle$ for fixed $r$ but any $\alpha$, i.e. These projection operators 
are a 1st step in finding the S.A.B.

These projection operators are defined by

$$\mathcal{P}^{(r)} = \frac{dr}{(\#G)} \sum_{g \in G} \chi^{(r)}(g)^* T(g)$$

---

A digression on projection operators in general. A proj. op. is specified 
by a subspace onto which it projects. The projection takes place $\perp$ 
to the subspace.

A proj. op has the properties:

$$\mathcal{P}^2 = \mathcal{P} \quad \text{(if you project twice, it's the same as}
\text{projecting once)}$$

$$\mathcal{P} = \mathcal{P}^* \quad \text{(this means the projection is $\perp$ to the subspace)}$$
A proj. op. has 2 eigenvalues, 0 and 1, and two corresponding eigenspaces. The eigenspace w. eigenvalue \( \neq 1 \) is the space upon which \( P \) projects. If \( x \) lies in this subspace, then \( Px = x \). The eigenspace w. eigenvalue 0 is the orthogonal subspace. If \( x \) lies in this subspace, then \( Px = 0 \).

To go back to the projection operators \( P^{(r)} \), we have a whole set of them, one for each \( r \) (it's not labeled).

First let's prove that \( P^{(r)} \) actually is a proj. op. Begin by showing it's Hermitian.

\[
P^{(r)^*} = \frac{dr}{(\# G)} \sum_{g \in G} \chi^{(r)}(g) T(g)^* \quad \text{Change variable of summation, } \quad h = g^{-1}
\]

\[
= \frac{dr}{(\# G)} \sum_{h \in G} \chi^{(r)}(h^{-1}) T(h) \quad \text{} \quad = tr M^{(r)}(h^{-1}) = tr M^{(r)}(h)^* = \chi^{(r)}(h)^*.
\]

\[
= \frac{dr}{(\# G)} \sum_{h \in G} \chi^{(r)}(h)^* T(h).
\]

Next, we'd like to show that \( P^{(r)^2} = P^{(r)} \). We can do something even more general, we will compute \( P^{(r)} P^{(s)} \).

\[
P^{(r)} P^{(s)} = \frac{dr ds}{(\# G)^2} \sum_{g \in G} \chi^{(r)}(g)^* \chi^{(s)}(gh)^* T(g) T(h) \quad \text{change variable of summation,} \quad a = gh, \quad h = g^{-1} a.
\]