MMP 2
Solutions 11

FS 19
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Exercise 1

C_{3v} has 3 conjugacy classes: $\{I\}, \quad \{C_3, {C_3}^2\}, \quad \{\sigma_v^{(1)}, \sigma_v^{(2)}, \sigma_v^{(3)}\}$

It is isomorphic to the dihedral group $C_{3v} \simeq D_3$: $\{\mathbf{1}\}, \quad \{R, R^2\}, \quad \{S, RS, R^2S\}$

a)

$$D_3 \xrightarrow{\sim} S_3, \quad R \mapsto \sigma \quad \text{s.t.} \quad R\vec{y}_i^* = \vec{y}_{\sigma(i)}^*, \tag{1}$$

where $y^* = (\vec{y}_1^*, \vec{y}_2^*, \vec{y}_3^*)$ are the equilibrium positions, forming a regular triangle.

> This is in fact a low number accident: the order of the dihedral group is $|D_n| = 2n$ and the one of the symmetric group is $|S_n| = n!$. So, in general they cannot be isomorphic. However, (1) always defines an isomorphism from D_n to a subgroup of S_n and for $n = 3$ the orders of the two groups coincide $|D_3| = 2 \cdot 3 = 6 = 3! = |S_3|$.

In the lecture (script p. 72) we used this isomorphism to define the representation ρ which operates on the $\vec{y}_i$ via the action of D_3 on $\mathbb{R}^2$ and undoes it for y^* by permuting the $\vec{y}_i^*$ with the inverse of the corresponding permutation:

$$\begin{array}{rccc} \rho: & C_{3v} & \to & GL((\mathbb{R}^2)^{\otimes 3}) \\ & R & \mapsto & (R\vec{y}_{\sigma^{-1}(1)}, R\vec{y}_{\sigma^{-1}(2)}, R\vec{y}_{\sigma^{-1}(3)}) \end{array}$$

Using (1) we see, that y^* is a fixed point of $\rho(R)$ $\forall R \in C_{3v}$:

$$\rho(R)y^* = (R\vec{y}_{\sigma^{-1}(1)}^*, R\vec{y}_{\sigma^{-1}(2)}^*, R\vec{y}_{\sigma^{-1}(3)}^*) = (\vec{y}_{\sigma(\sigma^{-1}(1))}^*, \vec{y}_{\sigma(\sigma^{-1}(2))}^*, \vec{y}_{\sigma(\sigma^{-1}(3))}^*) = y^*.$$

We use the matrix representation of S_3 on V^3 to write down the matrix forms of ρ for $\mathbf{1}, C_3$ and $\sigma_v^{(1)}$, which represent their conjucacy classes:

$$I \simeq id = (1), \qquad M(id) = \mathbb{1} \quad \Rightarrow \quad \rho(I) = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} \quad \Rightarrow \quad \chi_\rho(I) = 3\mathrm{Tr}(I) = 3 \cdot 2 = 6 = |C_{3v}|$$

$$C_3 \simeq \pi = (123), \qquad \rho(C_3) = C_3 \cdot M(\pi) = \begin{pmatrix} 0 & 0 & C_3 \\ C_3 & 0 & 0 \\ 0 & C_3 & 0 \end{pmatrix} \quad \Rightarrow \quad \chi_\rho(C_3) = 0$$

$$\sigma_v^{(1)} \simeq \tau = (12), \qquad \rho(\sigma_v^{(1)}) = \sigma_v^{(1)} \cdot M(\tau) = \begin{pmatrix} 0 & \sigma_v^{(1)} & 0 \\ \sigma_v^{(1)} & 0 & 0 \\ 0 & 0 & \sigma_v^{(1)} \end{pmatrix} \quad \Rightarrow \quad \chi_\rho(\sigma_v^{(1)}) = \mathrm{Tr}(\sigma_v^{(1)}) = 0$$

To determine the trace of $\sigma_v^{(1)}$ one can use the fact, that the trace is independent of the choice of basis and thus choose a comfortable matrix representation:
For example, let two points of the regular triangle be on the x-axis (y_1), while the third lies on the y-axis y_2. Then $M(\sigma_v^{(1)}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and thus $\mathrm{Tr}(M(\sigma_v^{(1)})) = \mathrm{Tr}(\sigma_v^{(1)}) = 0$.

b) Character table:

C_{3v}	I	$2C_3$	$3\sigma_v^{(1)}$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Projection formula:

$$n_{\rho_i} = \frac{1}{|G|} \sum_{g \in G} \overline{\chi_{\rho_i}(g)} \chi_\rho(g) = \frac{1}{|G|} \sum_K n_K \overline{\chi_{\rho_i}(k)} \chi_\rho(k), \quad k \in K$$

where n_{ρ_i} is the multiplicity with which the irreducible representation ρ_i appears in ρ and $n_K = |K|$ is the number of elements in the conjugacy class K.

$$\begin{aligned} n_{A_1} &= \frac{1}{6}\left(1 \cdot \overline{1} \cdot 6 + 2 \cdot \overline{1} \cdot 0 + 3 \cdot \overline{1} \cdot 0\right) = 1 \\ n_{A_2} &= \frac{1}{6}\left(1 \cdot \overline{1} \cdot 6 + 2 \cdot \overline{1} \cdot 0 + 3 \cdot (\overline{-1}) \cdot 0\right) = 1 \\ n_E &= \frac{1}{6}\left(1 \cdot \overline{2} \cdot 6 + 2 \cdot (\overline{-1}) \cdot 0 + 3 \cdot 0 \cdot 0\right) = 2 \end{aligned}$$

$$\Rightarrow \rho = \underline{A_1 \oplus A_2 \oplus E \oplus E}$$

c) The matrix $A = \left(m_i \frac{\partial^2 V}{\partial y_i^\alpha \partial y_j^\beta}(y^*)\right)_{i,j=1,2,3}^{\alpha,\beta=1,2}$ can be diagonalized and commutes with $\rho(R)$ $\forall R \in C_{3v}$. Thus, it has as many different eigenvalues as C_{3v} has irreducible representations and the dimensions of the eigenspaces coincide with the dimensions of the corresponding irreducible representations.

The rigid rotations correspond to A_2 and translations to E. Their eigenvalues are zero, since they move the entire system (without changing the distances between the atoms) and thus leave the potential invariant.
So, only A_1 and E remain and thus the subspace which has non-vanishing eigenvalues is given by $A_1 \oplus E$. $\Rightarrow$ $\underline{A \text{ has non-vanishing eigenvalues } \left\{ \begin{matrix} \lambda_{A_1} \\ \lambda_{E_2} \end{matrix} \right\} \text{ with multiplicity } \left\{ \begin{matrix} 1 \\ 2 \end{matrix} \right\}}$

Exercise 2

a)

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{=:N}$$

The matrix can be decomposed into a diagonal matrix D and a nilpotent matrix N with index 2: $N^2 = 0$.

$$\exp(tA) = \sum_{n=0}^{\infty} \frac{(tA)^n}{n!} = \sum_{n=0}^{\infty} \frac{t^n}{n!}(\mathbb{1} + N)^n = \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{k=0}^{n} \binom{n}{k} \mathbb{1}^{n-k} N^k = \sum_{n=0}^{\infty} \frac{t^n}{\cancel{n!}} \sum_{k=0}^{n} \frac{\cancel{n!}}{(n-k)!k!} N^k$$

$$\overset{N^2=0}{=} t + \sum_{n=1}^{\infty} t^n \left(\frac{1}{n!}\mathbb{1} + \frac{1}{(n-1)!} N \right) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathbb{1} + t \underbrace{\sum_{n=1}^{\infty} \frac{t^{n-1}}{(n-1)!}}_{n \mapsto n+1} N$$

$$= e^t \mathbb{1} + te^t N = \underline{\underline{e^t(\mathbb{1} + tN)}} = \underline{\underline{\begin{pmatrix} e^t & 0 & te^t \\ 0 & e^t & 0 \\ 0 & 0 & e^t \end{pmatrix}}}$$

b) $A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \Rightarrow \quad$ diagonalize it and use:

$$\exp(tA) = \exp(tTDT^{-1}) = \sum_{n=1}^{\infty} \frac{t^n}{n!} (\underbrace{TD\overbrace{T^{-1}T}^{\mathbb{1}}DT^{-1} \cdot \ldots \cdot TDT^{-1}}_{n \text{ times}}) = \sum_{n=1}^{\infty} \frac{t^n}{n!}(TD^nT^{-1}) = Te^{tD}T^{-1}$$

$$\det[A - \lambda\mathbb{1}] = \det \begin{pmatrix} 1-\lambda & 0 & 1 \\ 0 & 1-\lambda & 0 \\ 1 & 0 & -\lambda \end{pmatrix} = -\lambda(1-\lambda)^2 - (1-\lambda) = -(1-\lambda)[1 + \lambda(1-\lambda)] \overset{!}{=} 0$$

$$\Rightarrow \quad \lambda_1 = 1 \quad \text{and} \quad 1 + \lambda(1-\lambda) = -\lambda^2 + \lambda + 1 \overset{!}{=} 0 \quad \Rightarrow \quad \lambda_\pm = \frac{1 \pm \sqrt{5}}{2}$$

$$Eig(A,\lambda_1) = \ker(A-\lambda_1\mathbb{1}) = \ker\begin{pmatrix}0&0&1\\0&0&0\\1&0&-1\end{pmatrix} = \left\langle v_1 := \begin{pmatrix}0\\1\\0\end{pmatrix}\right\rangle$$

$$Eig(A,\lambda_\pm) = \ker(A-\lambda_\pm\mathbb{1}) = \ker\begin{pmatrix}\frac{1\mp\sqrt{5}}{2}&0&1\\0&\frac{1\mp\sqrt{5}}{2}&0\\1&0&-\frac{1\pm\sqrt{5}}{2}\end{pmatrix}$$

$$\Rightarrow \quad \begin{pmatrix}\frac{1\mp\sqrt{5}}{2}&0&1\\0&\frac{1\mp\sqrt{5}}{2}&0\\1&0&-\frac{1\pm\sqrt{5}}{2}\end{pmatrix}\begin{pmatrix}x_\pm\\0\\z_\pm\end{pmatrix} = \begin{pmatrix}\frac{1\mp\sqrt{5}}{2}x_\pm + z_\pm\\0\\x_\pm - \frac{1\pm\sqrt{5}}{2}z_\pm\end{pmatrix} \overset{!}{=} 0 \quad \Rightarrow \quad z_\pm = -\frac{1\mp\sqrt{5}}{2}x_\pm = \frac{2}{1\pm\sqrt{5}}x_\pm$$

This equation is satisfied $\forall x \in \mathbb{R}$ and we choose $x_\pm = \sqrt{\frac{2}{5\mp\sqrt{5}}}$ to normalize the eigenvectors:

$$Eig(A,\lambda_{2,3}) = \left\langle v_\pm := \sqrt{\frac{2}{5\mp\sqrt{5}}}\begin{pmatrix}1\\0\\-\frac{1\mp\sqrt{5}}{2}\end{pmatrix}\right\rangle$$

With the transformation matrix $T = (v_1, v_+, v_-)$ we can calculate the matrix exponential of tA:

$$\exp(tA) = T\begin{pmatrix}e^t&0&0\\0&e^{\frac{1+\sqrt{5}}{2}t}&0\\0&0&e^{\frac{1-\sqrt{5}}{2}t}\end{pmatrix}T^T = \begin{pmatrix}\frac{(5+\sqrt{5})e^{t\lambda_+}-(\sqrt{5}-5)e^{t\lambda_-}}{10}&0&\frac{e^{t\lambda_+}-e^{t\lambda_-}}{\sqrt{5}}\\0&e^t&0\\\frac{e^{t\lambda_+}-e^{t\lambda_-}}{\sqrt{5}}&0&\frac{(5+\sqrt{5})e^{t\lambda_-}-(\sqrt{5}-5)e^{t\lambda_+}}{10}\end{pmatrix}$$

$$= \underline{\underline{\frac{1}{2\sqrt{5}}\begin{pmatrix}(1+\sqrt{5})e^{t\lambda_+}-(1-\sqrt{5})e^{t\lambda_-}&0&2\left(e^{t\lambda_+}-e^{t\lambda_-}\right)\\0&2\sqrt{5}e^t&0\\2\left(e^{t\lambda_+}-e^{t\lambda_-}\right)&0&(1+\sqrt{5})e^{t\lambda_-}-(1-\sqrt{5})e^{t\lambda_+}\end{pmatrix}}}$$