HW2 Solution

① Problems 1 and 2. — please see lecture notes.

③ For D_{2n} group, there are $\{E\}$. $\{C_{2n}^1, C_{2n}^{2n-1}\}$, $\cdots$ $\{C_{2n}^n\}$, $\{Q.nC_2\}$, $\{nC_2'\}$, in total $n+3$ Classes. Hence, there should be $n+3$ irreducible representations, and $\underbrace{1^2+1^2+1^2+1^2}_{4} + \underbrace{2^2+\cdots 2^2}_{n-1} = 4n$

$\Rightarrow$ there are 4 1d representations, and $n-1$ 2d representations.

we first ~~construct~~ the 4 1d representations

A1 is the trival identity Rep.

A2 is the representation, which maps the C[illegible] normal subgroup to 1, and the other coset to -1.

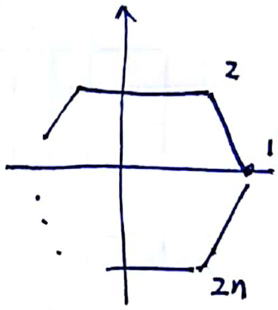
$B_{1,2}$ ~~is~~ carry the angular momentum n, ~~wh~~ but they are different under two different classes of in-plane rotations.

$E_{1,2,\cdots n-1}$, are 2D representations, carrying ~~ang~~ angular momentum $\pm1, \pm2, \cdots \pm(n-1)$, respectively. The ~~table~~ Character

	E	$2C_{2n}^1$	$2C_{2n}^2$	$\cdots$	$2C_{2n}^\ell$	$\cdots$	$2C_{2n}^{n-1}$	C_{2n}^n	nC_2	nC_2'
A_1	1	1	1	$\cdots$	1	$\cdots$	1	1	1	1
A_2	1	1	1	$\cdots$	1	$\cdots$	1	1	-1	-1
B_1	1	-1	1		$(-)^\ell$		-1	1	1	-1
B_2	1	-1	1		$(-)^\ell$		-1	1	-1	1

	E	$2C_{2n}^1$	$2C_{2n}^2$	$\cdots$	$2C_{2n}^l$	$\cdots$	C_{2n}^n	nC_2	nC_2'
E_1	2	$2\cos\frac{\pi}{n}$	$2\cos\frac{2\pi}{n}$	$\cdots$	$2\cos\frac{l\pi}{n}$	$\cdots$	-1	0	0
$\vdots$									
E_m	2	$2\cos\frac{m\pi}{n}$	$2\cos\frac{m2\pi}{n}$	$\cdots$	$2\cos\frac{ml\pi}{n}$	$\cdots$	$(-)^m$	0	0
$\vdots$									
E_{n-1}	2	$2\cos\frac{(n-1)\pi}{n}$	$2\cos\frac{2(n-1)\pi}{n}$	$\cdots$	$2\cos\frac{l(n-1)\pi}{n}$	$\cdots$	$(-)^{n-1}$	0	0

(4) Consider a $2n$-regular polygon, with n-vertices $|1\rangle, |2\rangle, \cdots |2n\rangle$. This form a $2n$-dimensional Reps



	E	$2C_{2n}^1$	$2C_{2n}^2$	$\cdots$ $2C_{2n}^l$	$\cdots$ C_{2n}^n	nC_2	nC_2'
χ	$2n$	0	0	0	0	2	0

$$\#\text{ of } A_1 = \frac{1}{|G|}\sum_g \chi_{A_1}^* \cdot \chi = \frac{1}{4n}(2n+2n) = 1$$

$$A_2 = \frac{1}{|G|}\sum_g \chi_{A_2}^* \cdot \chi = \frac{1}{4n}(2n-2n) = 0$$

$$B_1 = \frac{1}{|G|}\sum_g \chi_{B_1}^* \cdot \chi = \frac{1}{4n}(2n+2n) = 1$$

$$B_2 = \frac{1}{|G|}\sum_g \chi_{B_2}^* \chi = \frac{1}{4n}(2n-2n) = 1$$

Π:

$$E_l = \frac{1}{|G|}\sum_g \chi_{E_l}^* \chi = \frac{1}{4n}(2n\times 2) = 1$$

for $l = 1, 2, \cdots n-1$.

We can use angular momentum (discrete) to organize the molecular orbitals

① $m=0$ $\quad |\psi_0\rangle = \frac{1}{\sqrt{2n}} \sum_{i=1}^{2n} |i\rangle$ — A_1

② $m=n$ $\quad |\psi_n\rangle = \frac{1}{\sqrt{2n}} \sum_{i=1}^{2n} (-)^i |i\rangle$ — B_1

③ $\pm m =$ $\quad |\psi_\pm^{E_1}\rangle = \frac{1}{\sqrt{2n}} \sum_{j=1}^{2n} e^{\mp i \frac{2\pi}{2n}(j-1) m} |j\rangle$ — E_m, $\pm m = (\pm 1, \cdots \pm(n-1))$.

under this basis, the C_{2n}^{l} rotation is diagonal.

$$\begin{bmatrix} e^{-i\frac{\pi}{n}lm} & 0 \\ 0 & e^{i\frac{\pi}{n}lm} \end{bmatrix}$$

For C_2, around x-axis, $|1\rangle \to |1\rangle$, $|2\rangle \to |2n\rangle$, $|3\rangle \to |2n-1\rangle$, $\cdots$ $|n+1\rangle \to |n+1\rangle$

$C_2(\hat{x})|j\rangle = |2n+2-j\rangle \leftarrow$ in the sense mod $(2n)$

$$C_2(\hat{x})|\psi_+^{E_m}\rangle = \frac{1}{\sqrt{2n}} \sum_{j=1}^{2n} e^{-i\frac{\pi}{n}(j-1)m} |2n+2-j\rangle$$

$$= \frac{1}{\sqrt{2n}} \sum_{j'=1}^{2n} e^{-i\frac{\pi}{n}(2n+1-j')m} |j'\rangle = \frac{1}{\sqrt{2n}} \sum_{j'=1}^{2n} e^{i\frac{\pi}{n}(j'-1)m} |j'\rangle$$

$$= |\psi_-^{E_m}\rangle$$

Similarly $C_2(\hat{x})|\psi_-^{E_m}\rangle = |\psi_+^{E_m}\rangle \Rightarrow C_2(\hat{x}) : \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

For C_2 around the y-axis : $|1\rangle \to |n+1\rangle$, $|2\rangle \to |n\rangle$, $|3\rangle \to |n-1\rangle$

$\cdots\cdots$ $|2n\rangle \to |n+2\rangle$,

i.e $|j\rangle \to |n+2-j \ (\mathrm{mod}\ 2n)\rangle$

$$C_2(\hat{y})\,|\psi_+^{E_m}\rangle = \frac{1}{\sqrt{2n}} \sum_{j=1}^{2n} e^{-i\frac{\pi}{n}(j-1)m}\,|n+2-j\rangle$$

$$= \frac{1}{\sqrt{2n}} \sum_{j'=1}^{2n} e^{-i\frac{\pi}{n}(n+1-j')m}\,|j'\rangle = \frac{1}{\sqrt{2n}} \sum_{j'=1}^{2n} (-)^m\, e^{i\frac{\pi}{n}(j'-1)m}\,|j'\rangle$$

$$= (-)^m\,|\psi_-^{E_m}\rangle$$

Similarly $C_2(\hat{y})\,|\psi_-^{E_m}\rangle = (-)^m\,|\psi_+^{E_m}\rangle \Rightarrow C_2(\hat{y}) : \begin{pmatrix} 0 & (-)^m \\ (-)^m & 0 \end{pmatrix}$