Phys 220 Midterm Solution − C_{60}

5 1°: $H = \frac{L^2}{2I}$ where $I = mR^2$. Then the eigen-energy

$$E_l = \frac{\hbar^2 l(l+1)}{2mR^2}.$$

l is orbital angular momentum

degeneracy $(2l+1)\times 2$ by taking into accont spin ↑ and ↓

$l=5$ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ −

$l=4$ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓

$l=3$ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓

$l=2$ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓

$l=1$ ↑↓ ↑↓ ↑↓

$l=0$ ↑↓

2° $Y_h = Y \otimes \{E, I\}$, the Y group's character table is

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	E	$12C_5$	$12C_5^2$	$20C_3'$	$15C_2''$
A	1	1	1	1	1
T_1	3	$1+2\cos\frac{2}{5}\pi$	$1+2\cos\frac{4}{5}\pi$	0	−1
T_2	3	$1+2\cos\frac{4}{5}\pi$	$1+2\cos\frac{2}{5}\pi$	0	−1
G	4	−1	−1	1	0
H	5	0	0	−1	1

Y_h's representation will be A_u T_{1u} T_{2u} G_u and H_u

and A_g T_{1g} T_{2g} G_g and H_g

where u-represent odd parity and g-represent even parity

For spherical harmonics Y_{lm}. their characters for rotation angle θ

$$\chi^l(\theta) = \sin\left(\tfrac{1}{2}+l\right)\theta / \sin\theta/2$$

In lecture notes, we had the decomposition that

$$\boxed{\begin{array}{lll} s & - & A_g \\ p & - & T_{1u} \\ d & - & H_g \end{array} \qquad \begin{array}{lll} f & - & T_{2u} \oplus G_u \\ g & - & G_g \oplus H_g \\ h & - & T_{1u} \oplus T_{2u} \oplus H_u \end{array}}$$

Let us check $l=4$ and 5

l	E	$12C_5$	$12C_5^2$	$20C_3'$	$15C_2''$
4	9	-1	-1	0	1
5	11	1	1	-1	-1

g: $l=4$

$$\#\text{ of } G: \frac{1}{60}\left[4\times 9 + (-1)(-1)\times 12 + (-1)(-1)\times 12\right] = 1$$

$$\#\text{ of } H \quad \frac{1}{60}\left[5\times 9 + \cancel{(-1)(-1)\times 20} + (1)(+1)\times 15\right] = 1$$

even parity $\Rightarrow$ $g \rightarrow G_g \oplus H_g$

h: $l=5$

$$\#\text{ of } T_1: \frac{1}{60}\left[3\times 11 + \left(1+2\cos\tfrac{2}{5}\pi\right)\cdot 12 + \left(1+2\cos\tfrac{4}{5}\pi\right)\cdot 12 + (-)(-)\cdot 15\right] = 1$$

$$\#\text{ of } T_2: \quad 1$$

$$\#\text{ of } H: \frac{1}{60}\left[5\times 11 + (-)(-)\times 20 + (1)(-)\times 15\right] = 1$$

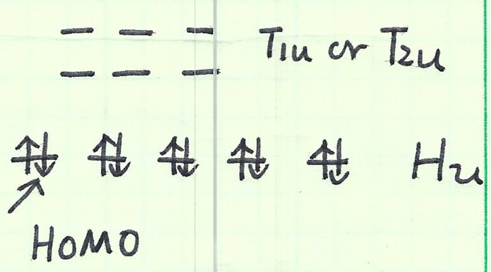
$\Rightarrow$ $h \rightarrow T_{1u} \oplus T_{2u} \oplus H_u$

The levels from $l = 0, 1, 2, 3, 4$ already taken 50 electrons

The last 10 electrons can occupy 5 levels, Hence the HOMO

should be $\boxed{H_u}$

$l = 5$ - - - - - - - - - - - - - $\longrightarrow$



3 The character of 60 dimensional Rep can be found be

7 Counting the number of fixed points

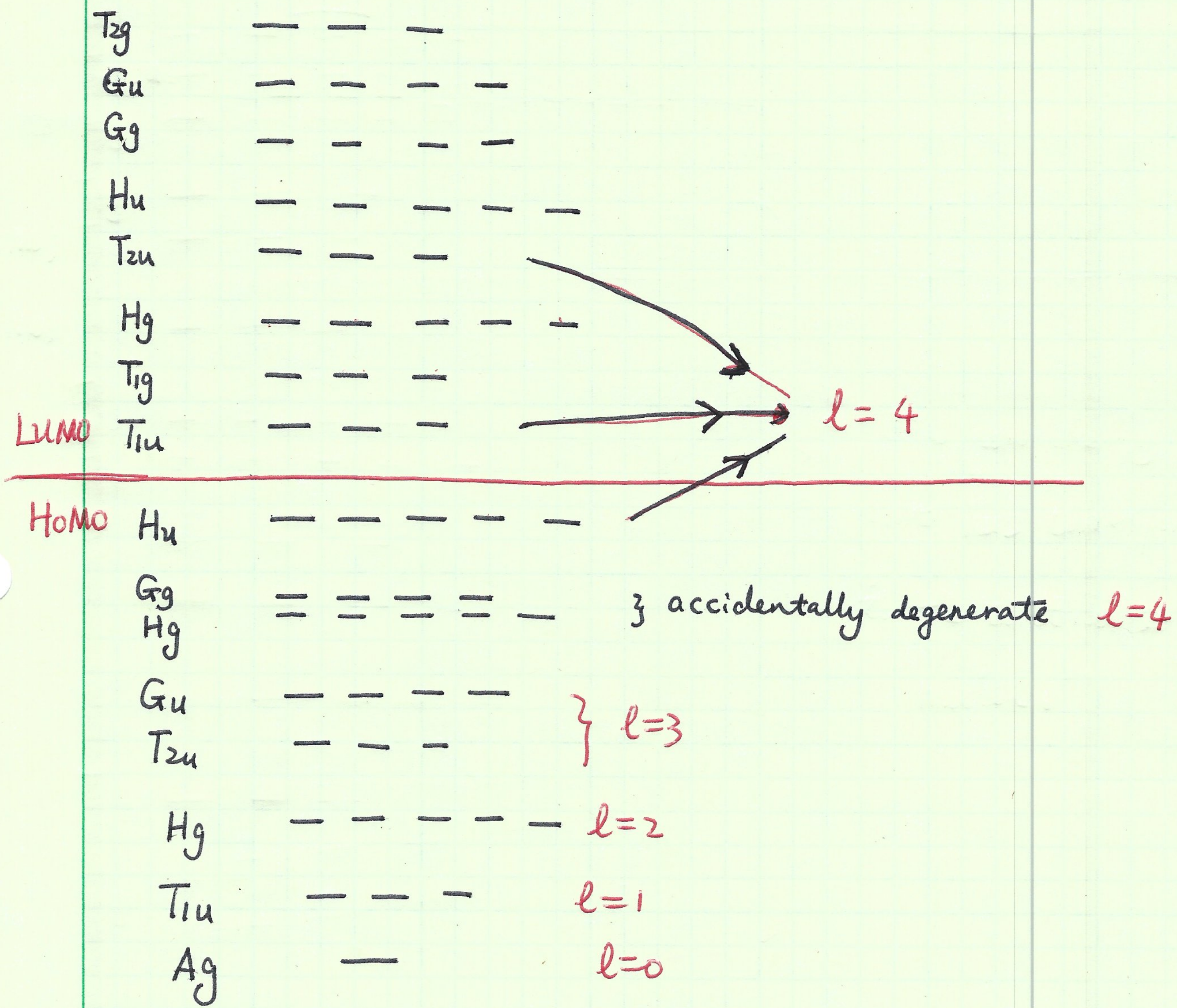
	E	$12C_5$	$12C_5^2$	$20C_3'$	$15C_2''$	I	$12IC_5$	$12IC_5^2$	$20IC_3'$	$15IC_2''$
χ	60	0	0	0	0	0	0	0	0	4

by calculating the characters with Y_h, we have

$$\chi = A_g \oplus T_{1g} \oplus T_{2g} \oplus 2G_g \oplus 3H_g$$

$$\oplus 2T_{1u} \oplus 2T_{2u} \oplus 2G_u \oplus 2H_u$$

④ By solving the 60 x 60 matrix for the tigh-binding model we should have the following sequence of energy levels



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5 For the vibration, we have 180 degrees of freedom.

	E	$12C_5^1$	$20C_3$	$12C_5^2$	$20C_2'$	I	$12IC_5^1$	$12IC_5^2$	$20IC_3$	15σ
χ	180	0	0	0	0	0	0	0	0	4

We can also make the inner product

$$\chi = 2A_g \oplus 4T_{1g} \oplus 4T_{2g} \oplus 6G_g \oplus 8H_g$$

$$\oplus A_{1u} \oplus 5T_{1u} \oplus 5T_{2u} \oplus 6G_u \oplus 7H_g$$

6 ~~So~~ too involved.

I will introduce you papers for this.