Disclaimer

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Marius Zache

A8.1

(1) $D_6 = \langle c, b \mid c^6 = e, b^2 = e, (bc)^2 = e \rangle$
$= \{e, c, c^2, c^3, c^4, c^5, b, bc, bc^2, bc^3, bc^4, bc^5\}$

Enough to check conj. classes w/ the generators?

For the conjugacy classes, we notice:

$[c^i] = \{g c^i g^{-1} \mid g \in D_6\}$

- $b c^i b = c^{n-i}$
- $b c^k c^i (bc^k)^{-1} = b c^k c^i c^{n-k} b = b c^{n+i} b = c^{-i}$

$[bc^i] = \{g\, bc^i g^{-1} \mid g \in D_6\}$

- $b\, b c^i b = b c^{n-i}$
- $c^k b c^i c^k = b c^{n-k} c^i c^k = b c^{n+i}$
- $(bc^k)(bc^i)(bc^k)^{-1} = b c^k b c^i c^{n-k} b = c^{n-k} c^i c^{n-k} b$
$= c^{n-k} c^i b c^k = c^{n-k} b c^{n-i} c^k = b c^k c^{n-i} c^k = b c^{2k-i}$

$\rightsquigarrow$ $[e] = \{e\}$ $\quad$ $[b] = \{b, bc^2, bc^4\}$
$[c] = \{c, c^5\}$ $\quad$ $[bc] = \{bc, bc^3, bc^5\}$
$[c^2] = \{c^2, c^4\}$
$[c^3] = \{c^3\}$

(2) For the number of irreducible representations, we use

$N_{irrep} = N_{cl} = 6$

For the dimensions, we use

$N_{D_6} = |\chi^1(e)|^2 + \ldots + |\chi^6(e)|^2$

$\rightsquigarrow 12 = d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2$

$\rightsquigarrow$ 2×2 dimensional irreps and 4×1 dimensional irreps

(3)

D_6	$[e]$	$\overset{1}{C_2}$ $[c^3]$	$\overset{2}{C_6}$ $[c]$	$\overset{2}{C_3}$ $[c^2]$	$\overset{3}{C_2}$ $[b]$	$\overset{3}{C_2}$ $[bc]$
1	1	1	1	1	1	1
1'	1	±1	±1	1	±1	±1
1''	1	±1	±1	1	±1	±1
1'''	1	±1	±1	1	±1	±1
2	2	^{a} ±2	^{c} ±1	^{x} ±1	^{w} 0	0
2'	2	^{b} ±2	^{d} ±1	^{y} ±1	^{z} 0	0

Why only integer numbers?

The first row and column can easily be filled

Orthogonality theorems:

- $\frac{N_{D_6}}{N_i}\delta^{ij} = \sum_{\nu=1}^{6} \chi^\nu(Cl_i)(\chi^\nu(Cl_j))^*$
- $N_{D_6}\delta^{\mu\nu} = \sum_{i=1}^{6} N_i \chi^\mu(Cl_i)(\chi^\nu(Cl_i))^*$

- We have $\chi(c^2) = \chi(c^4) = (\chi(c^2))^2 \rightsquigarrow \chi(c^2) = 1$

  as $\chi(c^2) \neq 0$: $\chi(c^2) = \chi(c^4) = (\chi(c^2))^{-1} \rightsquigarrow \chi(c^2) = \pm 1$

  for all 1 dim irreps.

$\Rightarrow 6 \overset{!}{=} 1^2+1^2+1^2+1^2+x^2+y^2 \rightsquigarrow x,y = \pm 1$

- $\chi(e) = \chi(b\cdot b) = \chi(b)\chi(b) \rightsquigarrow \chi(b) = \pm 1$ for 1 dim.

$\rightsquigarrow 4 = 1^2 + 3(\pm 1)^2 + w^2 + z^2 \rightsquigarrow w,z = 0$

- analogously for $\chi(e) = \chi(bc)\chi(bc)$
- For $\chi(e) = \chi(c^3)\chi(c^3) \rightsquigarrow \chi(c^3) = \pm 1$

  $12 \overset{!}{=} 1^2 + 3(\pm 1)^2 + a^2 + b^2 \rightsquigarrow a,b = \pm 2$
- $\chi(e) = \chi(c\cdot c^5) = \chi(c)\chi(c^5) \underset{\text{conj. cl.}}{\overset{\text{same}}{=}} \chi(c)\chi(c) \rightsquigarrow \chi(c) = \pm 1$

  $6 \overset{!}{=} 1^2 + 3(\pm 1)^2 + c^2 + d^2 \rightsquigarrow c,d = \pm 1$

$\Rightarrow$ table above

As the 3 * 1 dim. irreps are interchangeable, we just have to take care for the orthogonality theorems to be fulfilled really only 3 possibilities?

- A) $0 = 1 + 1 + 1 + 1 + 2x + 2y \rightsquigarrow x = y = -1$
- $0 = 1 + 2 + (\pm 1) + 2(\pm 1) + 3(\pm 1) + 3(\pm 1)$

$\rightsquigarrow$ 3 possibilities : $-1, -1, +1, -1$
$-1, -1, -1, +1$
$+1, +1, -1, -1$

D_6	$[e]$	$\overset{1}{[c^3]}$	$\overset{2}{[c]}$	$\overset{2}{[c^2]}$	$\overset{3}{[b]}$	$\overset{3}{[bc]}$
1	1	1	1	1	1	1
1'	1	-1	-1	1	1	-1
1''	1	-1	-1	1	-1	1
1'''	1	1	1	1	-1	-1
2	2	2	-1	-1	0	0
2'	2	-2	1	-1	0	0

- $0 = 2 + a + 2c - 2$ w/ $c = \pm 1, a = \pm 2$

$\rightsquigarrow$ 2 solutions

(4) $b = (6)(15)(24)(3)$, $c = (123456)$

$\rightsquigarrow c^2 = (123456)^2 = (135)(246)$

$c^3 = (14)(25)(36)$

$c^4 = (531)(642)$

$c^5 = (654321)$

$(bc) = (6)(15)(24)(3)(123456) = (41)(23)(56)$

$(bc^2) = (13)(5)(2)(46)$

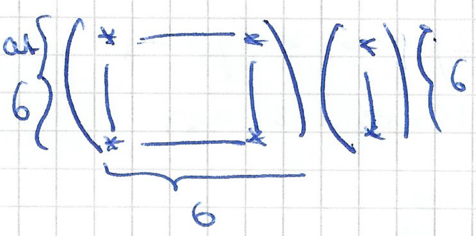
$(bc^3) = (12)(36)(45)$

$(bc^4) = (53)(1)(62)(4)$

$(bc^5) = (61)(25)(34)$

(5) For $[b] = \{b, bc^2, bc^4\}$, there are 2 atoms left at their positions, for the others none.

6) Looking at



, there are only entries on the diagonals, if an element is unchanged.

⇝ consider the 6-dim rep D^B of D_6 (as above)

⇝ $\chi^B(e) = 6$, $\chi^B([b]) = 2$, $\chi^B(\text{"else"}) = 0$

7) Consider $\frac{1}{N_{D_6}} \sum_{g \in D_6} |\chi^B(g)|^2 = \frac{1}{12}(3 \cdot 2^2 + 6^2) = 4 > 1$

⇝ is reducible

$D^B = \bigoplus_{\gamma} q_\gamma D^\gamma$ w/ $q_\gamma = \frac{1}{N_{D_6}} \sum_{i=1}^{N_{cc}} N_i (\chi^\gamma(\mathcal{C}_i))^* \cdot \chi(\mathcal{C}_i)$

$q_1 = \frac{1}{12}(3 \cdot 2 \cdot 1 + 1 \cdot 1 \cdot 6) = 1$

$q_{1'} = \frac{1}{12}(3 \cdot 2 \cdot 1 + 1 \cdot 1 \cdot 6) = 1$

$q_{1''} = \frac{1}{12}(3 \cdot 2(-1) + 1 \cdot 1 \cdot 6) = 0$

$q_{1'''} = \frac{1}{12}(3 \cdot 2(-1) + 1 \cdot 1 \cdot 6) = 0$

$q_2 = \frac{1}{12}(3 \cdot 2 \cdot 0 + 1 \cdot 2 \cdot 6) = 1$

$q_{2'} = \frac{1}{12}(3 \cdot 2 \cdot 0 + 1 \cdot 2 \cdot 6) = 1$

⇝ $D^B = q_1 + q_{1'} + q_2 + q_{2'}$

8) We have 4 states; 2 singlets and 2 doublets

Why can we say sth. about physics/spectrum if we are just working w/ math? No Hamiltonian considered?