PH563 Assignment 4

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Question 1.

(a) **3.**
This is the group $SO(2, 1)$ of Lorentz transformations. It has 3 generators, given by boosts along either of the axes, and rotation in the plane.

(b) $\sqrt{\frac{-2\hbar E}{\mu}}$.
We use the fact that the Lie bracket is bilinear, and substitute the given value of the scalar-free Lie Bbracket to obtain the desired expression for a.

(c) L_y.
The generators mentioned are given by

$$L_z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \text{ and } K_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and their commutator is easily calculated to be K_y, where in the same basis

$$K_y = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

(d) 12, 0, 2.
The characters are easily obtained by direct application of the required elements. The identity element preserves all coordinates, 12. The rotation does not preserve the position onf any atom, while the reflection preserves two.

(e) **22.**
The number of independent parameters in an $n \times n$ matrix is $2n^2$. The unitarity condition imposes a total of $\frac{n(n+1)}{2}$ constraints on this system (n^2 equations, and a strictly triangular part of size $\frac{n(n-1)}{2}$ removed, being identical due to adjoint invariance of the unitarity condition) remove the same number of independent parameters. Leaving us with $2n^2 - \frac{n(n+1)}{2}$ parameters, being 22 when evaluated for $n = 4$.

Question 2.

(a) iii. 9
The number of normal modes will be $2N$, and subtracting the 2 modes corresponding to translation and 1 of the rotation of the COM, we get $2N - 3$, which in our case, $N = 6$ is 9.

(b) iii. B_1
The normal coordinate corresponding to this mode is $x + y$, which corresponds to an eigenvector of $P_{B_1} - T_x$, and hence corresponds to the B_1 irreducible.

(c) none. $a = 2, b = 0, c = 1, d = 0$
We calculate the characters of the 4 conjugacy classes in the reducible representation, to get $\{3, 1, 1, 1\}$. Combined with the orthogonality relations, this gives us $\Gamma = 2A_1 \oplus B_1$.

Question 3.

(a) The symmetry group for the given figure is clearly C_{4v}. The character table for this group is

C_{4v}	E	$2C_4$(y)	C_2	$2\sigma_v$	$2\sigma_d$	basis
A_1	1	1	1	1	1	y
A_2	1	1	1	-1	-1	R_y
B_1	1	-1	1	1	-1	
B_2	1	-1	1	-1	1	
E	2	0	-2	0	0	$(x, z), (R_x, R_z)$

The characters for the classes in the columns, in order, would be, 8, as the identity preserves everything, 0, 0, and 0, since none of the reflections and rotations preserve the atoms' positions.

Using the character orthogonality relations, we get

$$\Gamma = A_1 \oplus A_2 \oplus B_1 \oplus B_2 \oplus 2E \ . \tag{1}$$

(b) Using the same process as in part a, we can calculate the decomposition, this time of course, using the character table of T_d instead.

$$\chi^{\Gamma^\alpha} = \{9, 0, 1, -1, 3\}$$

for the conjugacy classes $E, C_3, C_2, S_4, \sigma_d$.

And we get $\Gamma = A_1 \oplus A_2 \oplus B_1 \oplus B_2 \oplus 2E$.

(c) (i) The generators mentioned are given by

$$L_z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \text{ and } K_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and their commutator is easily calculated to be K_y, where in the same basis

$$K_y = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} .$$